Structure Analysis of Aluminum Hydride by the High Intensity Total Diffractometer (NOVA)

K. Ikeda[1], T. Otomo[1], H. Ohshita[1], N. Kaneko[1], M. Tsubota[1], T. Seya[1], K. Suzuya[2], H.-W. Li[3], S. Semboshi[3], S. Orimo[3], on behalf of NOVA group
[1]IMSS KEK, [2]J-PARC Center JAEA, [3]IMR Tohoku Univ.

A high-intensity total diffractometer, NOVA, at J-PARC realizes new opportunity to explore structures of hydrogen storage materials. NOVA can observe crystalline structure as well as amorphous and liquid structure in a short time, and clarify the structural changes during hydriding and dehydriding reactions of the hydrogen storage materials.

Aluminum trihydride (AlH_3, alane) is one of the potential candidates for hydrogen storage materials because of high gravimetric and volumetric hydrogen densities (10 mass% and 149 kgH_2/m^3, respectively) and a simple dehydriding reaction ($AlH_3 \rightarrow Al + 3/2H_2$) at 370–470 K [1–3]. We investigated the dehydriding reaction of AlH_3 by *in situ* microscopic observations combined with thermal, surface and atomic structural analyses [4–7]. Before the dehydriding reaction, primary AlH_3 particles of size 100 nm–1 μm were covered by an oxide layer of thickness 3–5 nm. Both the precipitation/grain-growth of metallic Al of size 1–50 nm and an increase in boundary space were clearly observed inside the particles, while the morphologies of the particles covered by the layer did not change during the dehydriding reaction. Moreover, the presence of χ-Al_2O_3 on the surface was suggested by the high-intensity neutron/X-ray diffraction measurements. In the paper, details of the synthesis process, dehydriding reactions depending on temperatures and structural analysis are presented.

[1] G. Sandrock et al., *Appl. Phys. A*, 80 (2005) 687; [2] J. Graetz, and J.J. Reilly, *J. Phys. Chem. B*, 109 (2005) 22181; [3] S. Orimo et al., *Appl. Phys. A*, 83 (2006) 5; [4] K. Ikeda et al., *Nanotechnology*, 20 (2009) 204004; [5] S. Muto et al., *J. Appl. Phys.*, 105 (2009) 123514; [6] S. Kato et al., *Appl. Phys. Lett.*, 96 (2010) 51912; [7] K. Ikeda et al., *Mater. Trans.*, submitted.